## Center for Nanoscale Control of Geologic CO_2 (NCGC)
EFRC Director: Donald J. DePaolo
Lead Institution: Lawrence Berkeley National Laboratory

Mission Statement: *To build a fundamental understanding of molecular-to-pore-scale processes in fluid-rock systems, and to demonstrate the ability to control critical aspects of flow, transport, and mineralization in porous rock media as applied to the injection and storage of carbon dioxide (CO_2) in subsurface reservoirs.*

Technical Overview: The vision for the Center is to understand, predict, and enhance the performance of underground CO_2 storage systems. Specific goals are to (1) establish novel molecular, nanoscale, and pore-network scale approaches for controlling flow, dissolution, and precipitation in deep subsurface rock formations to achieve efficient filling of pore space with injected supercritical CO_2, with maximum solubility- and mineral trapping and near-zero leakage, and (2) develop a predictive capability for the fate of injected CO_2 that is applicable for a 1000 years into the future. Our focus is

at the nano- to pore scale where subsurface processes originate from chemical and physical interactions. The word "control" in the title has a double meaning – it connotes an effort to better understand how nanoscale processes control larger scale processes, and, more heroically, to use such information to optimize storage of injected CO_2.
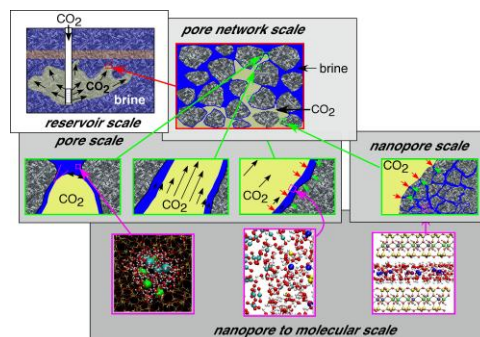
The NCGC consists of a team of highly qualified investigators with expertise in, and access to, the most advanced analytical and computing facilities available for furthering fundamental knowledge of the nanoscale properties and processes of CO_2-brine-mineral systems. Our primary objective is not to provide specific engineering parameters for a subsurface storage system, but to raise understanding of fluid-rock processes to a new level using a coordinated and focused research effort. Although we expect the new knowledge we generate to be useful for applications other than CO_2 storage, the unique character of the NCGC derives from its focus on supercritical CO_2 and its behavior and fate in subsurface reservoirs, and the scale and coordination of the research effort.

The NCGC is focused on three aspects of geologic carbon sequestration:
1. Understand and enhance mineralization of injected CO_2
2. Optimize the performance of geologic traps and seals
3. Understand and optimize reservoir fluid-rock reactive transport processes

Our largest effort (Thrust Area 1) is on understanding how carbonate minerals nucleate and precipitate under the conditions of CO_2 sequestration in both reservoir rocks (e.g. sandstones) and geologic seals (shales). This emphasis follows from the fact that in many reservoir rocks, there is sufficient cation supply to mineralize most of the CO_2, but the release rate of cations by dissolution is slow and hence the long-term system performance is uncertain. Thrust 1 also capitalizes on the rapid progress being made on molecular scale understanding of mineral dissolution and precipitation processes stimulated by the tools available at the DOE light sources, computing centers, and nanoscience and technology centers. The remainder of the NCGC effort (Thrust Areas 2 and 3) is focused on the properties of fluid mixtures under confinement in high-surface area environments, and the interplay between flow and chemical reactions; the latter involves understanding the geometrical relationships between CO_2, brine, and minerals, and the mechanisms by which mineral fluid-reactions are affected by the unique features of the two-phase (or 3-phase) fluid system. Thrusts 2 and 3 include key computational research tasks, and

unique opportunities afforded by the neutron facilities at ORNL. The nanoscale processes involved in CO_2 sequestration are first aggregated at the pore scale (μm to mm). Thrust Area 3 is focused on pore scale and multi-scale heterogeneity effects on CO_2 trapping.
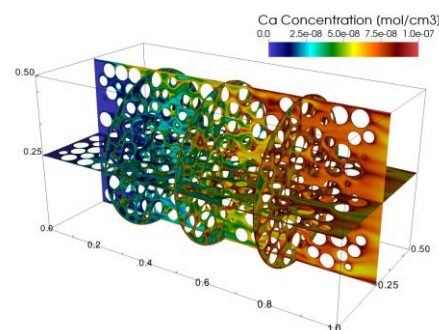
Mineral-fluid reactivity: Thrust Area 1 aims to provide an understanding of the molecular scale mechanisms and materials parameters that govern the processes of dissolution and precipitation under reservoir conditions, with the ultimate goal of establishing the upscaled parameters that will enable accurate modeling of reservoir- wide evolution, and the scientific basis for engineering approaches to enhancing CO_2 trapping processes.
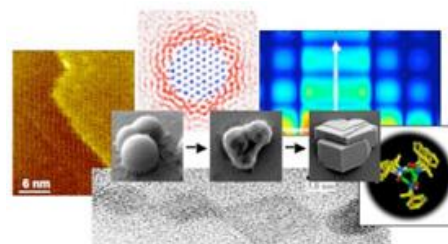
Nanopore Processes: Thrust Area 2 focuses on properties of confined fluids, a key issue relevant to the behavior of caprocks and the reactivity of reservoir rocks. A related issue is the wetting properties of minerals, which arise from molecular-scale properties of fluid-fluid and fluid-solid interfaces and is essential to predicting the capillary pressure curves of reservoir rocks and caprocks, properties that strongly influence the efficiency of reservoirs and the security of caprocks. Wetting contrasts also produce thin films on minerals, which vary with changes in mineralogy, pore water chemistry, or other conditions, and strongly affect the long-term distribution and reactivity of CO_2.
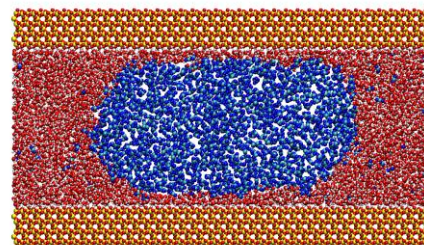
Pore-Scale Processes: Thrust Area 3 investigates "emergent processes" associated with the injection of CO_2 into the deep subsurface, which forces the subsurface system far from equilibrium, where a range of self-organizing processes can lead to emergent, time-dependent structures. Our focus is on structures that emerge due to process coupling at the pore scale, since this is ultimately the framework within which the fluids migrate and/or reside and minerals dissolve and precipitate.   This research is bringing to bear a new generation of experimental, imaging and modeling tools specifically designed to address pore scale dynamics.

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